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EXCITATION OF ATOMS BY ELECTRON BOMBARDMENT

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Brief survey of recent literature on the excitation probability of atoms by electron bombardment. Approximate formulas for the effective cross sections of atom excitation by electron bombardment are derived on the basis of simple considerations. The formulas are shown to yield cross section estimates of an accuracy of a factor of 1.5 to 3.

In the present report we will examine the approximation of a formula for effective cross sections of atomic excitation by electron bombardment, derived on the basis of simple considerations and permitting a ready estimate of the cross section to within a factor of 1.5 - 3.

I. Let us begin with Born's well-known formula which corresponds to a representation of the wave function of the "atom + electron" system as the simple product of a plane wave and the function describing the atom, and has the form:

$$\sigma_{ab} = \frac{8\pi}{K_a^2} \int_{K_a-K_b}^{K_a+K_b} \left| \left\langle b \left| \sum_{j=1}^{N} e^{iqr_j} \right| a \right\rangle \right|^2 \frac{dq}{q^3}. \qquad (1)$$

Here, a and b are sets of quantum numbers denoting the initial and final states of the atom and $q = K_a - K_b$ is the transferred momentum. We will use atomic units. Figure 1 shows several examples, encompassing a rather broad range of change in absolute magnitudes of cross sections from $0.03\ \pi a_0^2$ for He to $50\ \pi a_0^2$ for Na.

We see from the graphs that in the high-energy collision region, i.e., where the Born formula can be considered well-substantiated, calculation and experiment give quite close results.

If, despite this fact, a noticeable divergence occurs it apparently must be explained by the insufficiently accurate measurement of the absolute values of cross sections in the experiment or, perhaps, by the use of insufficiently accurate atomic functions in the calculations. If in such cases the theoretical and experimental curves coincide at high energies, then on the whole the agreement becomes quite homogeneous. In the region of the cross-section maximum, the Born approximation proves to be overestimated by a factor of 1.5 to 3. Thus, this

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approximation can be used whenever such an error is acceptable; however, for many problems more accurate results are desirable. /3

Furthermore, the Born formula does not permit calculating the transition probabilities accompanied by a variation in atomic spin. Such transitions, just as is the case for exchange corrections for transitions without a variation in spin, can be calculated only with consideration of the inherent symmetry properties of the wave function. The Born-Oppenheimer formula used for this purpose, as was indicated by one of us earlier (Ref.1), is not correct, which explains the poor quality of results obtained by means of it. In the same paper, we stated that the correct expression for the amplitude of exchange scattering, g_{ab}, has the form

$$g_{ab} = -\frac{4}{K_a^2} \left\langle b \left| \sum_{j=1}^{N} e^{iqr_j} \right| a \right\rangle. \qquad (2)$$

In Fig.2 we present several curves illustrating the quality of calculations which can be performed by means of this formula. As indicated in the graph, it has approximately the same degree of accuracy as calculations for nonexchange transitions.

Therefore, at present almost all rules for improving the "Bornian" results actually or simply follow the line of satisfying two requirements:

a) An "improved theory" should lead to cross sections that agree with the known inequalities ensuring conservation of the number of particles in scattering

$$\sigma_{ab}^{(L)} \leq \frac{\pi}{K_a^2} (2L + 1) \qquad (3)$$

where $\sigma_{ab}^{(L)}$ is the L-th partial cross section.

b) The obtained cross sections should be below the "Bornian". For lack of space, we will not dwell on the various means of cutting off total and partial cross sections as they had been proposed for achieving these purposes, especially since such methods as the use of the R matrix (Ref.2, 3) or the method of the collision parameter (Ref.4, 5), in our opinion, rather have the character of a general rule and, in essence, do not extend beyond the frame of the Born approximation.

Therefore, we will discuss more fully only the paper by L.Vaynshteyn, L.Presnyakov, and I.Sobel'man (Ref.6) in which an attempt is made to use an initial approximation for the wave function that is more accurate than that used in the Born method. The basic idea here is that, with respect to the problem of atomic excitation, a major role is played by the interaction of free and atomic electrons which should be taken into account as completely as possible. /4 Examining the problem of the hydrogen atom, the authors assume

$$\psi(r_1, r_2) = e^{ikr_1} \varphi(r_1, r_2) \qquad (4)$$

where the function $\varphi(r_1, r_2)$ is selected such that it accurately describes the electron-electron scattering and the motion of their common center of mass in the field of the nucleus. Although the specific form of the function $\varphi(r_1, r_2)$ is rather complex, a substitution of eq.(4) into the integral identity for the scattering amplitude makes it possible to continue all necessary calculations which lead to the following formula:

$$\sigma_{ab} = \frac{8\pi}{K_a^2} \int_{K_a - K_b}^{K_a + K_b} |\langle b|e^{iqr}|a\rangle|^2 [f(\nu, x)]^2 \frac{dq}{q^3} \qquad (5)$$

where

$$f(\nu, x) = \frac{\pi\nu}{\sinh \pi\nu} F(-i\nu, i\nu, 1, x)$$

$$x = \left[\frac{\Delta\varepsilon + q^2}{\Delta\varepsilon + 3q^2}\right]^2; \quad \nu = K_a^{-1}; \quad \Delta\varepsilon = K_a^2 - K_b^2$$

while F(a, b, c, x) is a hypergeometric function.

Thus, eq.(5) differs from Born's formula (1) only by the factor f(v, x) which tends to unity for large collision energies. A generalization of these formulas for the case of a complex atom is given elsewhere (Ref.7). Figure 3 shows the results of the calculations performed for transitions $1s$–$2s$ and $1s$–$2p$ in hydrogen and $5s$–$5p$ and $5s$–$6p$ in rubidium. We see from the diagram that, whenever a comparison with the experiment is possible, the results are quite satisfactory.

II. As stated before, the results of the first approximation may be too rough, especially when the plasma temperature is not very high and when it is not the maximal value of the excitation probability that is of interest but its values near the threshold. Often, they are even more unsatisfactory, namely, when it is necessary to obtain the transition probabilities between states of similar energy, mainly between excited states. In these problems, the results of calculations performed in first approximation often contradict the principle of conservation of the number of particles.

Unfortunately, progress in the development of more accurate methods of calculation is hampered by the fact that the various hypotheses made for this purpose cannot be anywhere near completely substantiated, or even estimated, within the frame of the theory itself. Experimental data on the absolute values of cross sections usually are of insufficient accuracy and, in the case of /5 transitions between excited states, are virtually nonexistent.

III. Although the above-mentioned methods of calculating cross sections are rather simple, their use requires knowledge of the atomic functions and of computer work, which latter is readily done on electronic computers; without computers, however, the problem is not too simple. Therefore, simplified formulas proposed for a rapid estimation of the probabilities of allowed transitions may be of interest, especially since the results obtained by their aid in the /6

low-energy region need not be inferior in accuracy to the results of more complex calculations.

Expanding, in the Born formula $\exp(iqr)$, in a power series and limiting ourselves to a dipole approximation we arrive at the Bethe formula

$$\sigma_{ab} = \frac{2\pi f_{ab}}{(\Delta E_{ab})^2} \cdot \frac{\Delta E}{E} \ln(3E) \qquad (6)$$

which indicates that the cross section is mainly determined by the factor $\frac{2\pi f_{ab}}{(\Delta E_{ab})^2}$, where f_{ab} is the force of the oscillator and ΔE_{ab} is the excitation energy.

Concrete calculations performed in the Born approximation show that, for a large number of transitions, the cross sections expressed in threshold units $x = \left(\frac{E - \Delta E_{ab}}{\Delta E_{ab}}\right)^{1/2}$ behave in like manner. They reach a maximum when $x = 1 - 2$, and the maximal value of the cross section itself, in fact, is quite satisfactorily transferred by the indicated factor. This permits proposing the following semiempirical formula for describing the excitation function:

$$\sigma_{ab} = \frac{2\pi f_{ab}}{(\Delta E_{ab})^2} P(x) \qquad (7)$$

where $P(x)$ can be selected, for example, in the form of $C_1 \frac{4x^2}{(1 + x^2)^2} \ln(C_2 x)$ where C_1 and C_2 are constants of the order of unity. Details on the selection of $P(x)$ and the result of averaging the values of $v\sigma$ according to the Maxwellian distribution can be found elsewhere (Ref.8).

A similar approach was proposed by M.Seaton (Ref.2). Seaton, considering that the functions $P(x)$ change little from atom to atom, proposed to construct these functions from experimental data for such different atoms as He, H, and Na and, being convinced that the derived curves are actually quite close, suggested their use in calculations for other atoms. According to the author's assertion, the error of the results obtained in this manner will not exceed 100%.

These methods, although quite simple, nevertheless require knowing the force of the oscillator of the transition in question. Furthermore, good estimates can be made with the use of only the values of the energy levels of the atom.

We mentioned above that the interaction of free and atomic electrons plays a principal role in the problem of atomic excitation. But the cross section for the transmission of energy ε from one electron to another, if we disregard the effect of the nucleus, can be obtained very simply and, in the case where the

atomic electron is considered to be at rest, has the form:

$$d\sigma = \frac{\pi}{E} \cdot \frac{d\varepsilon}{\varepsilon^2}. \tag{8}$$

If now we assume, by definition, that the excitation of the n-th level of the atom occurs when ε satisfies the inequality $E_n \leq \varepsilon \leq E_{n+1}$ (where E_n is the excitation energy of the n-th level), then, for the excitation cross section, we obtain

$$\sigma_e = N \cdot \frac{\pi}{E} \begin{cases} E_n^{-1} - E^{-1} & E_n \leq E \leq E_{n+1} \\ E_n^{-1} - E_{n+1}^{-1} & E \geq E_{n+1} \end{cases} \tag{9}$$

and, for the ionization cross section

$$\sigma_i = N \cdot \frac{\pi}{E} (E_j^{-1} - E^{-1}) \tag{10}$$

where N is the number of electrons in the valence shell of the atom. This latter is known as the Thomson formula.

In this form, these formulas yield the proper estimate for the absolute values of the excitation cross section of the group of levels lying in the given energy range. However, the maximum itself proves to be too sharp and approaches the threshold too closely; at high energies, the cross section is noticeably underestimated. Recently, various attempts were made to improve /8 these results (Ref.9, 10, 11) but it seems that the most correct approach lies not in complicating the calculations but in constructing semiempirical formulas of the type of eq.(7) by using eqs.(9) or (10) as the scale factor.

Thus, Drawin (Ref.12) found that the formula

$$\sigma = 0.66\, \sigma_i \cdot C_1 \ln\left(1.25 \cdot C_2 \frac{E}{E_j}\right) \tag{11}$$

satisfactorily describes the ionization functions. It was shown elsewhere (Ref.13) that the same formula, on substituting σ_i from eq.(10) by σ_e from eq.(9), just as satisfactorily describes the excitation. Figure 4 illustrates the obtained results.

It should be noted that eq.(8), forming the basis of these calculations cannot - because of the very meaning of its derivation - lead to such misunderstandings as the nonconservation of the number of particles in scattering; therefore, calculations performed by its aid may even be preferable over Born's method, especially for transitions between excited states.

In conclusion, we repeat that we investigated only certain methods of calcu-

lation that yield an estimate of the absolute values of the cross sections and truly impart a general form to the excitation functions. We disregarded not only problems of a further quantitative refinement of the theory but also certain qualitative problems such as the existence of resonance maxima and minima on excitation functions. As is known, such characteristics are found experimentally in elastic scattering and should exist in inelastic scattering also.

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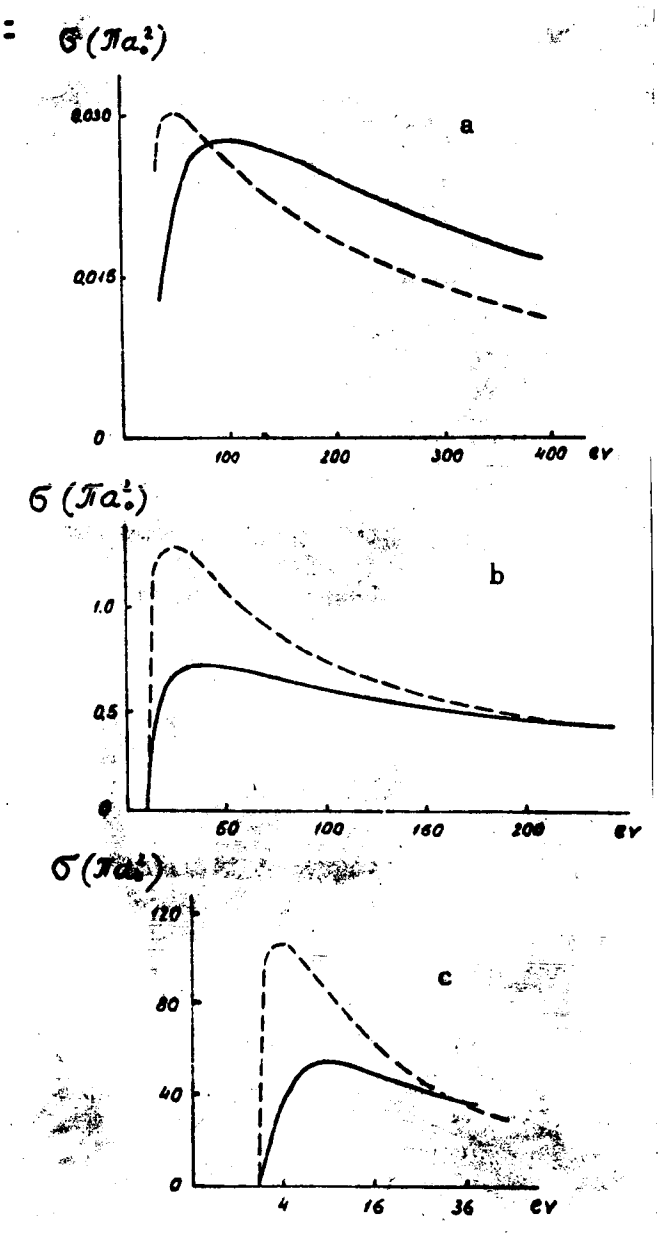

Fig.1

a - Transition $1s-3\,{}^1p$ in He
b - Transition $1s-2p$ in H
c - Transition $3s-3p$ in Na

Solid curve - experiment; dashed curve - Born approximation.

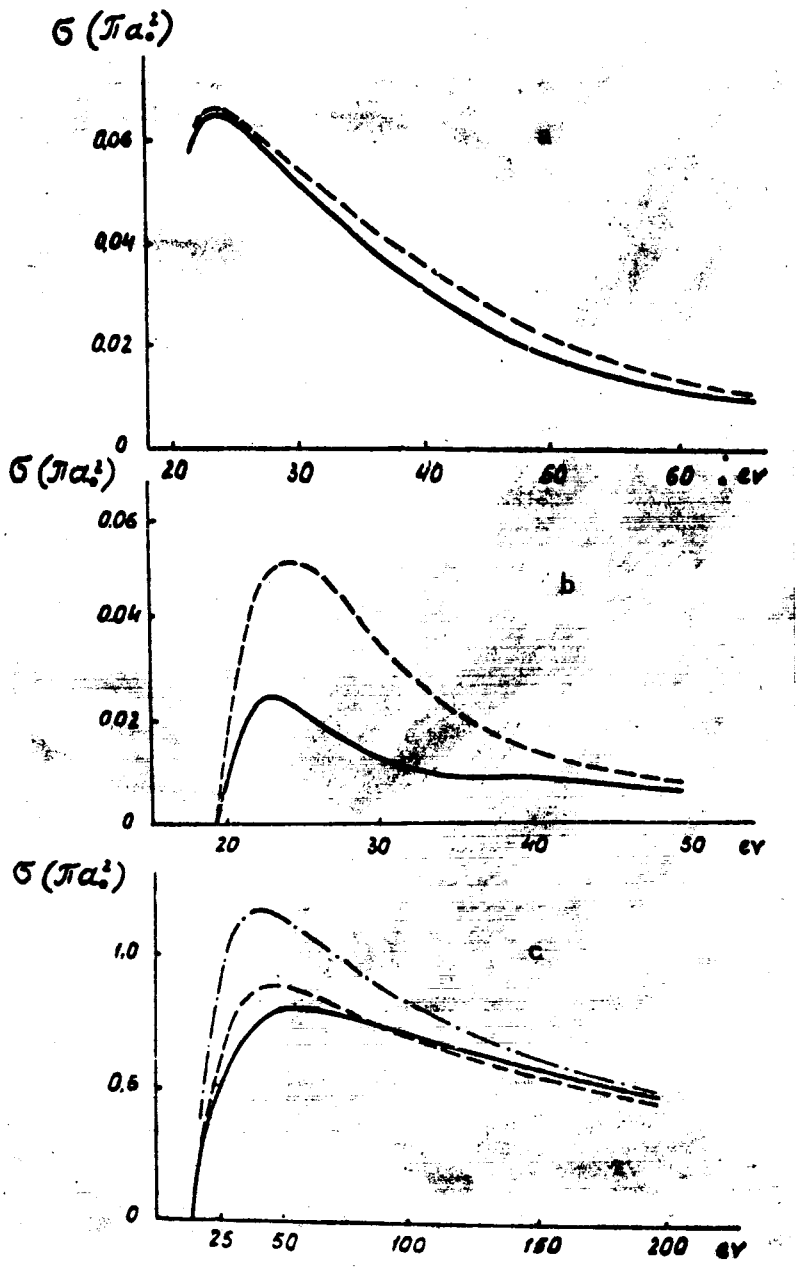

Fig.2

a - Transition 1s–2 ^{3}S in He
b - Transition 1s–2 ^{3}P in He
c - Ionization of H

Solid curve - experiment; dashed curve - calculation by eq.(2); dot-dash curve - calculation in Born approximation.

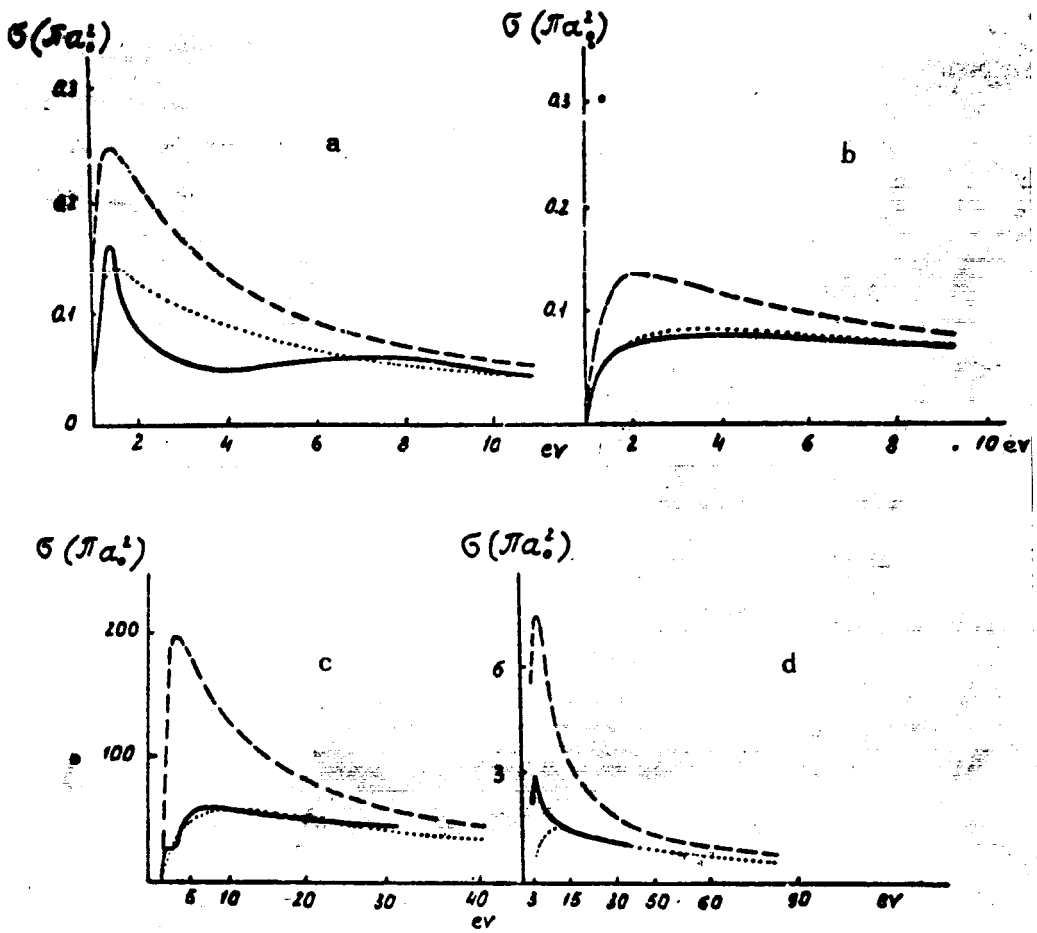

Fig.3

a - Transition 1s–2s in H
b - Transition 1s–2p in H
c - Transition 5s–5p in Rb
d - Transition 5s–6p in Rb

Solid curve - experiment; dashed curve - Born approximation;
dots - calculation by eq.(5).

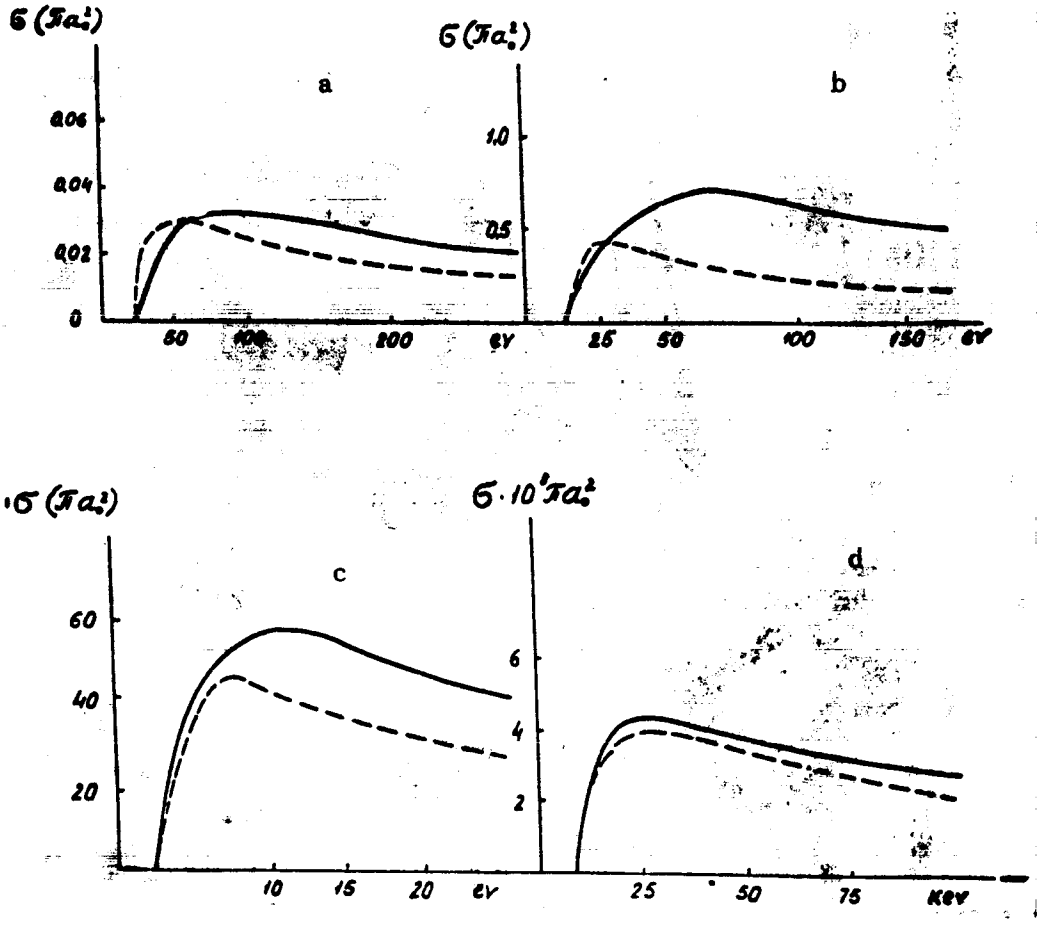

Fig.4

a - Transition 1s-3 ^{1}P in He
b - Transition 1s-2p in H
c - Transition 3s-3p in Na
d - Ionization of K-shell of Ni

Solid curve - experiment; dashed curve - calculation by eqs.(9), (11).

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